

Zero-energy states and fragmentation of spin in the easy-plane antiferromagnet on a honeycomb lattice

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The core of the vortex in the Néel order parameter for an easy-plane antiferromagnet on honeycomb lattice is demonstrated to bind two zero-energy states. Remarkably, a single electron occupying this mid-gap band has its spin fragmented between the two sublattices: Whereas it yields a vanishing total magnetization it shows a finite Néel order, orthogonal to the one of the assumed background. The requisite easy-plane anisotropy may be introduced by a magnetic field parallel to the graphene's layer, for example. The results are relevant for spin-1/2 fermions on graphene's or optical honeycomb lattice, in the strongly interacting regime.

The fact that the low-energy quasiparticles in graphene behave as massless Dirac fermions has placed this new incarnation of carbon-based structures at the center stage of condensed-matter physics [1]. Although in its natural state graphene appears to be a gapless semimetal, it is tempting to also consider it in its possible strongly correlated phases, where the quasiparticles would become gapped and the ground state insulating. Such a semimetal-insulator transition in graphene would in fact represent a condensed-matter analog of the Higgs mechanism, with the Higgs field as a quasiparticle composite [2], [3]. Although the ultimate nature of the insulating phase that would result from the strong Coulomb interaction may depend on the details at the scale of the lattice constant, the simplified Hubbard model on a honeycomb lattice is most likely to have the standard Néel-ordered ground state at a sufficiently large U/t . This is certainly what is expected at $U/t = \infty$, and is also supported by numerical [4] and analytical [3] studies, already for U/t above some critical value.

As long as the quantum phase transition between the semimetal and the antiferromagnetic insulator is not strongly discontinuous and not too deep in the insulating phase, it is still sensible to consider fermions as itinerant. Weak antiferromagnetic ordering is then felt by the formerly gapless quasiparticles as an opening of a “relativistic” mass gap, with the “mass” being proportional to the Néel order parameter. The unusual universality class of this transition is completely determined by the presence of gapless Dirac fermions on the semimetallic side [3]. It seems natural to ask if there could be other interesting consequences of this fact in the insulating phase itself. In particular, in light of the known properties of the spectrum of Dirac's Hamiltonian in topologically non-trivial backgrounds [5], [6] one wonders if topological defects in the Néel order here may localize sub-gap states at zero energy. Such states have been known to display a number of unusual features, such as charge fractionalization [5], [6] and non-abelian statistics [7] and are being discussed intensively in the context of topological quantum computing [8].

I show here that this is indeed the case at least when there is an easy-plane anisotropy for the Néel order, when the core of the vortex in the order parameter turns out to

contain a pair of such mutually orthogonal zero-energy states. The electric charge of the vortex in this case is integer; however, the core states have the positional and spin degrees of freedom entangled in an interesting way. At half filling, this two-state mid-gap band is half full. A single electron occupying the zero-energy band then has the direction of its spin alternating between the two triangular sublattices of the honeycomb lattice. Its spin after averaging over the unit cell therefore vanishes. Its Néel order parameter, however, is finite, and points in the direction orthogonal to the easy-plane. An electron occupying the zero-energy state would thus represent a local *single-particle antiferromagnet*. Placing the system in a weak magnetic field parallel to the graphene layer is further demonstrated to introduce such an easy-plane anisotropy for the Néel ordering. This may help create the experimental conditions for an observation of this effect in graphene's or optical honeycomb lattice.

Let us begin by defining the standard Hubbard model as $H_t + H_U$, with

$$H_t = -t \sum_{\vec{A}, i, \sigma = \uparrow, \downarrow} u_{\sigma}^{\dagger}(\vec{A}) v_{\sigma}(\vec{A} + \vec{b}_i) + H.c., \quad (1)$$

$$H_U = U \sum_{\vec{X}} n_{\uparrow}(\vec{X}) n_{\downarrow}(\vec{X}). \quad (2)$$

The sites \vec{A} denote one triangular sublattice of the hexagonal lattice, generated by linear combinations of the basis vectors $\vec{a}_1 = (\sqrt{3}, -1)(a/2)$, $\vec{a}_2 = (0, a)$. The second sublattice is then at $\vec{B} = \vec{A} + \vec{b}$, with the vector \vec{b} being either $\vec{b}_1 = (1/\sqrt{3}, 1)(a/2)$, $\vec{b}_2 = (1/\sqrt{3}, -1)(a/2)$, or $\vec{b}_3 = (-a/\sqrt{3}, 0)$. a is the lattice spacing, and $U > 0$.

The spectrum of H_t for each projection of spin becomes linear in the vicinity of the two non-equivalent Fermi points, which we choose to be at $\pm \vec{K}$, with $\vec{K} = (1, 1/\sqrt{3})(2\pi/a\sqrt{3})$ [9]. In vicinity of these points the linearized Hamiltonian assumes a “relativistically invariant” form $H_0 = \gamma_0 \gamma_i \partial_i$ with $\gamma_0 = I_2 \otimes \sigma_3$, $\gamma_1 = \sigma_3 \otimes \sigma_2$, $\gamma_2 = I_2 \otimes \sigma_1$, where $\{I_2, \vec{\sigma}\}$ is the standard Pauli basis. The global “chiral” SU(2) symmetry for each spin projection is generated by $\{\gamma_{35}, \gamma_3, \gamma_5\}$, where $\gamma_3 = \sigma_1 \otimes \sigma_2$, $\gamma_5 = \sigma_2 \otimes \sigma_2$, and $\gamma_{35} = i\gamma_3\gamma_5 = \sigma_3 \otimes I_2$

[10]. In the continuum limit, the four-component wavefunction for each spin projection is given by $\Psi_\sigma^\dagger(\vec{x}) = (u_{1\sigma}^\dagger(\vec{x}), v_{1\sigma}^\dagger(\vec{x}), u_{2\sigma}^\dagger(\vec{x}), v_{2\sigma}^\dagger(\vec{x}))$, where

$$u_{i\sigma}(\vec{x}) = \int^\Lambda \frac{d\vec{q}}{(2\pi a)^2} e^{-i\vec{q}\cdot\vec{x}} u_{1\sigma}((-)^{i+1}\vec{K} + \vec{q}), \quad (3)$$

and analogously for $v_{i\sigma}(\vec{x})$. The “valley” index $i = 1, 2$ labels the two Fermi points. The reference frame has been rotated so that $q_x = \vec{q} \cdot \vec{K}/K$ and $q_y = (\vec{K} \times \vec{q}) \times \vec{K}/K^2$, and $\hbar = k_B = v_F = 1$, where $v_F = ta\sqrt{3}/2$ is the Fermi velocity.

The interaction term H_U can also be written as

$$H_U = \frac{U}{16} \sum_{\vec{A}} [(n(\vec{A}) + n(\vec{A} + \vec{b}))^2 + (n(\vec{A}) - n(\vec{A} + \vec{b}))^2 (4 - (\vec{f}(\vec{A}) + \vec{f}(\vec{A} + \vec{b}))^2 - (\vec{f}(\vec{A}) - \vec{f}(\vec{A} + \vec{b}))^2)],$$

where $n(\vec{A}) = u_\sigma^\dagger(\vec{A})u_\sigma(\vec{A})$ and $\vec{f}(\vec{A}) = u_\sigma^\dagger(\vec{A})\vec{\sigma}_{\sigma\sigma'}u_{\sigma'}(\vec{A})$, are the particle number and the magnetization operators at the site \vec{A} . Variables at the second sublattice are analogously defined in terms of $v_\sigma(\vec{B})$. This is the rotationally invariant version of the decomposition previously introduced in [3].

Assume next that the ground state has a uniform average density, zero average magnetization, and finite Néel order: $\langle n(\vec{x}) \rangle = n$, $\langle \vec{f}(\vec{A}) + \vec{f}(\vec{A} + \vec{b}) \rangle = 0$, $\vec{N} = \langle \vec{f}(\vec{A}) - \vec{f}(\vec{A} + \vec{b}) \rangle \neq 0$. For the Hubbard model we believe this to be the leading instability of the semi-metallic ground state above critical U/t [3]. By the usual Curie-Weiss decoupling the last term in Eq. (4) yields then the mean-field Hamiltonian for the Dirac fermions in a fixed Néel background $\vec{N}(\vec{x})$:

$$H_N = I_2 \otimes H_0 - (\vec{N}(\vec{x}) \cdot \vec{\sigma}) \otimes \gamma_0, \quad (5)$$

with the first operator in the direct product acting on the spin, and the second on the Dirac indices. For example, if $\vec{N}(\vec{x}) = (0, 0, N)$ and constant, in the ground state of H_N the average number of spin-up (spin-down) electrons is larger on the sublattice B (A). The ground state of H_N exhibits therefore a uniform Néel ordering along the third spin axis in this case. Since all three γ -matrices appearing in H_0 are diagonal in valley indices, one can rewrite $H_N = H_1 \oplus H_2$, with

$$H_{1(2)} = \pm I_2 \otimes \sigma_1 (-i\partial_1) + I_2 \otimes \sigma_2 (i\partial_2) - (\vec{N}(\vec{x}) \cdot \vec{\sigma}) \otimes \sigma_3 \quad (6)$$

as the intra-valley Hamiltonians near the Fermi points at \vec{K} (H_1), and $-\vec{K}$ (H_2). Both H_1 and H_2 on the other hand may be recognized as unitary transformations of the generic Hamiltonian H : $H = H_0 + \vec{m}(\vec{x}) \cdot \vec{M}$, where $\vec{M} = (i\gamma_0\gamma_3, i\gamma_0\gamma_5, \gamma_0)$. Specifically, $H_1 = U_1^\dagger H U_1$, with

$$U_1 = I_2 \oplus i\sigma_2 \quad (7)$$

and $\vec{m}(\vec{x}) = (N_1(\vec{x}), N_2(\vec{x}), -N_3(\vec{x}))$, and $H_2 = U_2^\dagger H U_2$, with

$$U_2 = i\sigma_2 \oplus I_2 \quad (8)$$

and $\vec{m}(\vec{x}) = (N_1(\vec{x}), N_2(\vec{x}), N_3(\vec{x}))$. H represents the most general single-particle Hamiltonian in two dimensions with the relativistic spectrum $E^2 = k^2 + m^2$ and with the chiral symmetry of H_0 broken [11]. It may also be understood as the mean-field Hamiltonian for spinless particles on a honeycomb lattice in the background of the order parameter $\vec{m} = \langle \Psi^\dagger \vec{M} \Psi \rangle$. For instance, $\vec{m} = (0, 0, m)$ is the familiar state with a density imbalance between the A and B sublattices [9], [12], [3], whereas $\vec{m} = (m_1, m_2, 0)$ represents a state with broken translational symmetry, with the “Kekule” pattern of hopping integrals of different magnitudes [6].

Finding the spectrum of H_N is therefore a special case of the general problem of diagonalizing H for a given configuration of the mass matrix $\vec{m}(\vec{x})$. Here I focus on the issue of zero-energy states for the vortex configuration. Assume that one of the components of $\vec{m}(\vec{x})$ vanishes everywhere, say $m_3(\vec{x}) = 0$. As a result, $\{\gamma_0, H\} = 0$. Since $\gamma_0^2 = 1$, $\gamma_0 = P_+ - P_-$ where P_\pm are the projectors onto two orthogonal eigenspaces corresponding to ± 1 eigenvalues. This, on the other hand, means that when $m_3(\vec{x}) = 0$, $H = P_+ H P_- + P_- H P_+$, so that H is block-off-diagonal in the eigenbasis of γ_0 in which $P_+ = I_2 \oplus 0$ [13]. For γ_0 as defined right below Eq. (1) this change of basis amounts to a simple exchange of the second and the third components of $\Psi(\vec{x})$. Next, assume that $\Delta = m_1(\vec{x}) + im_2(\vec{x}) = |\Delta(r)|e^{ip\phi}$, $p = \pm 1$, is the vortex configuration, with (r, ϕ) as polar coordinates and, and $|\Delta(r \rightarrow \infty)| \rightarrow m$. This problem was considered by Jackiw and Rossi [14] and recently by Hou et al [6]. Defining $\partial_z = \partial_x + i\partial_y$, the zero-energy state $\Psi_0(\vec{x})$ satisfies either

$$i\partial_z v(\vec{x}) + \Delta^* v^*(\vec{x}) = 0, \quad (9)$$

with $v_1 = v_2^* = v(\vec{x})$ and $u_1 = u_2 = 0$, or

$$i\partial_z u(\vec{x}) + \Delta^* u^*(\vec{x}) = 0 \quad (10)$$

with $u_1 = u_2^* = u(\vec{x})$, and $v_1 = v_2 = 0$. For $p = 1$ one finds:

$$v(\vec{x}) = \frac{C}{r} e^{-i\phi} f(r), \quad (11)$$

with $u = 0$ and $-\ln f(r) = \int_0^r |\Delta(t)| dt + i(\pi/4)$, and

$$u(\vec{x}) = C f(r) \quad (12)$$

with $v = 0$. C is the normalization factor. Only the second solution is normalizable, however, and thus represents the unique zero-energy eigenstate of H . The situation is reversed for an antivortex, when $p = -1$. For general p one can show that there are $|p|$ linearly independent zero-energy bound states.

An important general property of the zero-energy states should be noted. Consider the following sum:

$$q(\vec{x}) = \sum_{E \in R} \Psi_E^\dagger(\vec{x}) Q \Psi_E(\vec{x}), \quad (13)$$

where Q is a traceless Hermitean matrix, and $\{\Psi_E(\vec{x})\}$ the eigenstates of the generic Hamiltonian H . If the summation is performed over the whole spectrum, $q(\vec{x}) \equiv 0$. If R includes only the occupied states, on the other hand, the sum represents the ground-state average of a physical observable, $\langle q(\vec{x}) \rangle$. By subtracting a half of the vanishing sum over the whole spectrum one can rewrite this same average as [15]

$$\langle q(\vec{x}) \rangle = \frac{1}{2} \left(\sum_{\text{occup}} - \sum_{\text{unoccup}} \right) \Psi_E^\dagger(\vec{x}) Q \Psi_E(\vec{x}). \quad (14)$$

The last form makes it evident that if there exists a unitary matrix T that anticommutes with H , for any Q that commutes with T the only states that can contribute to $\langle q(\vec{x}) \rangle$ are the states with zero energy. For the vortex Hamiltonian considered above, $T = \gamma_0$. Choosing $Q = \gamma_0$ yields then $\langle q(\vec{x}) \rangle = \langle m_3(\vec{x}) \rangle$, whereas for $Q = i\gamma_0\gamma_3$, $\langle q(\vec{x}) \rangle = \langle m_1(\vec{x}) \rangle$ for example. The important observation is that the contribution to the hard-axis component of the order parameter comes *exclusively* from the zero-energy state.

We now translate these results to the vortex in the Néel order. Take the Néel vector to be in the plane 1-2: $\vec{N} = (N_1(\vec{x}), N_2(\vec{x}), 0)$, with $\Delta(\vec{x}) = N_1(\vec{x}) + iN_2(\vec{x}) = |\Delta(r)|e^{i\phi}$. The zero-energy eigenvalue of H_1 is then

$$\Psi_{1,0} = \begin{pmatrix} u_{1\uparrow} \\ v_{1\uparrow} \\ u_{1\downarrow} \\ v_{1\downarrow} \end{pmatrix} = U_1^\dagger \Psi_0 = f(r) \begin{pmatrix} 1 \\ 0 \\ 0 \\ i \end{pmatrix}, \quad (15)$$

and of H_2 ,

$$\Psi_{2,0} = \begin{pmatrix} u_{2\uparrow} \\ v_{2\uparrow} \\ u_{2\downarrow} \\ v_{2\downarrow} \end{pmatrix} = U_2^\dagger \Psi_0 = f(r) \begin{pmatrix} 0 \\ 1 \\ i \\ 0 \end{pmatrix}, \quad (16)$$

with $f(r)$ assumed to be normalized. The two zero-energy states are degenerate, orthogonal, and exponentially localized at the center of the vortex. Consider a linear combination $\Psi^\dagger = a^*(\Psi_{1,0}^\dagger, 0) + b^*(0, \Psi_{2,0}^\dagger)$, $|a|^2 + |b|^2 = 1$. In this state,

$$u_\uparrow(\vec{x}) = ae^{i\vec{K}\cdot\vec{x}}f(r), \quad (17)$$

$$u_\downarrow(\vec{x}) = ibe^{-i\vec{K}\cdot\vec{x}}f(r), \quad (18)$$

and

$$v_\uparrow(\vec{x}) = be^{-i\vec{K}\cdot\vec{x}}f(r), \quad (19)$$

$$v_\downarrow(\vec{x}) = iae^{i\vec{K}\cdot\vec{x}}f(r). \quad (20)$$

where $w_\sigma = w_{1\sigma}e^{i\vec{K}\cdot\vec{x}} + w_{2\sigma}e^{-i\vec{K}\cdot\vec{x}}$, $w = u, v$. Introducing $u^\dagger = (u_\uparrow^*, u_\downarrow^*)$ and $v^\dagger = (v_\uparrow^*, v_\downarrow^*)$, the average particle

densities on the sublattices A and B in the state Ψ are equal to

$$u^\dagger u = v^\dagger v = |f(r)|^2, \quad (21)$$

independently of the state Ψ . The average of the third component of the spin, on the other hand, is

$$u^\dagger \sigma_3 u = -v^\dagger \sigma_3 v = (|a|^2 - |b|^2)|f(r)|^2, \quad (22)$$

and thus *alternating* between the two sublattices. For the easy-plane components of the average spin we can compactly write,

$$-iu^\dagger \sigma_+ u = iv^\dagger \sigma_- v = 2a^* b e^{-2i\vec{K}\cdot\vec{x}} |f(r)|^2, \quad (23)$$

which is evidently zero for both $\Psi = \Psi_{1,0}$ and $\Psi = \Psi_{2,0}$ [16].

Exactly at half-filling the two-state band at zero-energy is occupied by a single electron, which is in some arbitrary state Ψ . Whereas in any such state the electron has an equal probability to be found on either sublattice, the projection of its spin along *any* axis when integrated over the whole system is zero [17]. However, unless $|a| = |b|$, the electron spin will manifest itself in the *staggered* magnetization in the direction orthogonal to the plane of the Néel background. Taking into account the zero-states' local contribution to the order parameter the vortex would thus be turned into a half-skyrmion. It is a remarkable property of the zero-energy states that the spin of a single electron is distributed in such an alternating pattern. It agrees, however, with the observation on the general nature of the zero-energy states made earlier.

As shown below, one way of introducing such an easy plane for the Néel order parameter is to turn on a uniform magnetic field and couple it to particle's spin. It is of interest therefore to understand how that would perturb the zero-energy states. In the zero-energy subspace spanned by $(\Psi_{1,0}^\dagger, 0)$ and $(0, \Psi_{2,0}^\dagger)$ the Zeeman term is represented by the perturbation

$$H_Z = \lambda(\sigma_3 \otimes I_2) \oplus (\sigma_3 \otimes I_2), \quad (24)$$

where $\lambda = -\mu_B B$. It is obvious that $\langle \Psi_{i,0} | H_Z | \Psi_{j,0} \rangle = 0$, and there is no shift in energies to the first order in B . Physical reason is precisely the states' vanishing magnetization, which decouples them from the magnetic field to the first order.

The energies do shift, however, if the Néel vector is tilted out of the easy plane. Assume a configuration $\vec{N} = (N_1(\vec{x}), N_2(\vec{x}), N_3)$, with $N_1(\vec{x}) + iN_2(\vec{x}) = |\Delta(r)|e^{i\phi}$ as before, but with a uniform $N_3 \ll |\Delta(\infty)|$. Within the two-dimensional zero-energy subspace this perturbation is represented by

$$H_3 = -N_3(\sigma_3 \otimes \sigma_3) \oplus (\sigma_3 \otimes \sigma_3). \quad (25)$$

This gives $\langle \Psi_{i,0} | H_3 | \Psi_{j,0} \rangle = \pm N_3 \delta_{ij}$. A finite component N_3 at half filling would therefore force one of the states

in Eqs. (15)-(16) to be occupied and the other one to be empty.

Let us show how the Zeeman coupling to the magnetic field introduces easy-plane anisotropy for the Néel order in the present case. To this purpose add the term $\lambda(\sigma_3 \otimes I)$ to H_N in Eq. (5), and assume a uniform \vec{N} . The third spin axis, of course, may be in an arbitrary direction in the real space. Decomposing the new Hamiltonian again as right above Eq. (6), one now finds H_1 and H_2 as unitary transforms of $H + \lambda\gamma_{35}$, with the eigenstates [18]:

$$E(k) = \pm[(\sqrt{N_3^2 + k^2} \pm |\lambda|)^2 + (N_1^2 + N_2^2)]^{1/2}. \quad (26)$$

In the ground state at half filling all the negative energy states are occupied and the positive energy states empty. It is easy to show then that among all possible orientations of \vec{N} the lowest energy belongs to the one with $N_3 = 0$. An obvious way to enforce such a purely Zeeman coupling would be to orient the magnetic field parallel to the plane of the honeycomb lattice. The Néel order parameter would then be confined to the plane orthogonal to the honeycomb lattice.

Hou et al. [6] have recently found zero-energy states on graphene's honeycomb lattice in the spectrum of spinless electrons in the vortex in their two-component "Kekule" order parameter, as discussed below Eq. (8). In that case there is a single zero-energy state, a remarkable consequence of which is that the charge of a vortex that binds it is fractionalized. In contrast, since we have two zero-

energy states, the charge of each is simply unity, but it is the spin properties of the states that are nontrivial. The crucial feature of our example, however, is that the relevant $U(1)$ symmetry of the order parameter is the exact rotational symmetry. This makes one cautiously optimistic about the survival of the mid-gap states once the lattice effects are fully restored. In this context it would be particularly interesting to diagonalize the lattice version of H_N numerically. A related recent calculation [19] shows zero-energy states to be surprisingly resilient to the effects of the discrete lattice.

In conclusion, the mean-field Hamiltonian for Dirac quasiparticles in the background of a vortex in weak Néel order on graphene's honeycomb lattice has two orthogonal core states at zero energy, with positional and spin degrees of freedom maximally entangled. An electron in one of these states at half filling is a single-particle antiferromagnet with a finite, localized contribution to the staggered magnetization in the direction orthogonal to the easy plane, and zero average magnetization. The required easy-plane anisotropy was shown to be introduced by placing the graphene layer in a weak parallel magnetic field.

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 - [16] Furthermore, since the continuum limit is meaningful only if $|\Delta(r)|$ is a slowly varying function on the scale of the lattice spacing, the easy-plane components in Eq. (23) vanish even if $a^*b \neq 0$ due to the rapidly oscillating prefactor. As the single length scale in H is v_F/m , this requires the mass-gap to be small compared to the bandwidth, and the system thus to be close to a (nearly) continuous semimetal-insulator phase transition.
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